

Degenerate approach to the mean field Bose- Hubbard Hamiltonian

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A degenerate variant of mean field perturbation theory for the on-site Bose-Hubbard Hamiltonian is presented. We split the perturbation into two terms and perform exact diagonalization in the two-dimensional subspace corresponding to the degenerate states. The final relations for the second order ground state energy and first order wave function do not contain singularities at integer values of the chemical potentials. The resulting equation for the phase boundary between superfluid and Mott states coincides with the prediction based on the conventional mean field perturbation approach.

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The bosonic Hubbard model has been the subject of intense theoretical interest [1–3]. It describes quantum phase transition between the superfluid and Mott phases of ultracold bosonic atoms in an optical lattice, first realized in experiment by *Greiner et al.* [4]. A qualitatively correct phase diagram of the model at zero temperature can be captured by a simple mean field theory [5–10]. This theory predicts superfluid phase for non-integer fillings and a transition to an insulating Mott phase for integer fillings. This findings were confirmed with numerical calculations (quantum Monte Carlo simulation) [11–13], variational approach [14], cluster Gutzwiller method [15], and more elaborate analytical methods, including strong-coupling perturbation theory [16], slave-boson theory [17–19], effective action approach [20–22], random phase approximation [23–25], bosonic dynamical mean-field theory [26], multisite mean-field theory [27–29], higher-order series expansions [30, 31].

In this paper, we present an alternative estimation of the zero-temperature ground state wave function $|\psi_{gs}\rangle$ and energy E_{gs} , which takes into account the degenerate character of the ground state of H_0 at integer values of the chemical potential μ . The resulting formulas for $|\psi_{gs}\rangle$ and E_{gs} are free from singularities which otherwise are present at integer values of the chemical potentials in the conventional perturbative mean field approach [10].

For this we perform first the diagonalization of the on-site mean-field Hamiltonian in the basis of the two lowest states at a given μ , and the account for the rest of the perturbation by a conventional technique. The properties of the Mott phase and the superfluid phase in a Hilbert space restricted to the number-basis states $|n\rangle$ and $|n+1\rangle$ (the corresponding Gutzwiller state is $\prod_i |\psi\rangle_i$, with $|\psi\rangle = f_n|n\rangle + f_{n+1}|n+1\rangle$) was considered in Refs. [32, 33].

In the framework of mean field approach the hopping term between sites i and j is decoupled as, $b_i^\dagger b_j \simeq \langle b_i^\dagger \rangle b_j + b_i^\dagger \langle b_j \rangle - \langle b_i^\dagger \rangle \langle b_j \rangle$ and the Bose- Hubbard (BH) Hamiltonian is reduced to on-site Hamiltonian $H = H_0 + H_t$,

$$H_0 = -\mu_0 n + \frac{U_0}{2} n(n-1), \quad (1)$$

$$H_t = -t_0 \nu (\psi^* b + \psi b^\dagger) + t_0 \nu |\psi|^2, \quad (2)$$

where U_0 is a repulsive on-site boson- boson interaction,

H_t is the mean field kinetic energy, t_0 is the nearest-neighbor hopping amplitude, ν is the number of nearest neighbors. The symbols b and b^\dagger denote destruction and creation operators for bosons at a lattice site, $\psi = \langle b \rangle$ is the order parameter, $n = b^\dagger b$ is the boson number operator. The chemical potential μ_0 controls the average number of bosons.

It is convenient to rewrite H in dimensionless units $\mu_0/U_0 = \mu$, $t_0 \nu/U_0 = t$ and $H/U_0 = h$. In these units

$$h = h_0 + h_t + t|\psi|^2, \quad (3)$$

$$h_0 = -\mu n + \frac{1}{2} n(n-1), \quad h_t = -t(\psi^* b + \psi b^\dagger) \quad (4)$$

Eigenfunctions of h_0 are the number states $|n\rangle$ and eigenvalues are $\varepsilon_n = n^2/2 - (\mu + 1/2)n$, $n = 0, 1, 2, \dots$. The ground state of h_0 , $|\psi_{gs}^{(0)}\rangle = |n\rangle$, $E_{gs}^{(0)} = \varepsilon_n$, corresponds to the number of bosons n if the chemical potential μ is in the range $n-1 < \mu < n$. At integer values of μ the ground state is two-fold degenerate: $\varepsilon_n = \varepsilon_{n+1}$, $|\psi_{gs}^{(0)}\rangle = \{|n\rangle, |n+1\rangle\}$ at $\mu = n$, and $\varepsilon_{n-1} = \varepsilon_n$, $|\psi_{gs}^{(0)}\rangle = \{|n-1\rangle, |n\rangle\}$ at $\mu = n-1$.

The usual practice to handle the perturbation h_t is numerical diagonalization of h in the subspace spanned by the vectors $|n\rangle$, $n = 0, 1, \dots, n_{max}$. This approach essentially equivalent to the formulation based on the Gutzwiller wave function $|\psi\rangle = \prod_i \sum_{n=0}^{n_{max}} f_n^{(i)} |n\rangle_i$, see Refs. [2, 8, 15, 34].

Another method is a perturbative treatment of the hopping term. Corrections to the ground state wave function and energy in the framework of standard non-degenerate perturbation theory [10, 35] are

$$\begin{aligned} |\psi_{gs}\rangle &= |\psi_{gs}^{(0)}\rangle + |\psi_{gs}^{(1)}\rangle = \\ &= |n\rangle + \left[\frac{(-t)\psi^* \sqrt{n}}{n-1-\mu} |n-1\rangle + \frac{(-t)\psi \sqrt{n+1}}{\mu-n} |n+1\rangle \right], \end{aligned} \quad (5)$$

$$E_{gs} = \varepsilon_n + t|\psi|^2 \left(1 - t\chi_0(\mu, n) \right), \quad (6)$$

$$\chi_0(\mu, n) = \left[\frac{n+1}{n-\mu} + \frac{n}{\mu-n+1} \right], \quad (7)$$

where the value of the chemical potential is considered to be in the interval $n - 1 < \mu < n$.

The zero-temperature phase boundary between the Mott state, $|\psi| = 0$, and the superfluid state, $|\psi| > 0$, corresponds to the vanishing of the coefficient of the $|\psi|^2$ -term of the expansion of the energy functional $E_{gs}(\psi)$, which gives the equation $1 = t\chi_0(\mu, n)$. The resulting line of critical values of t as a function of μ is

$$t(\mu, n) = \frac{1}{\chi_0(\mu, n)} = \frac{(n - \mu)(\mu - n + 1)}{1 + \mu}, \quad (8)$$

Although expression for $\chi_0(\mu, n)$, Eq. (7), is not defined close to the integer values of μ , the quantity $1/\chi_0(\mu, n)$ well behaves at integer μ and, as a result, the boundary curve, Eq. (8), safely includes $\mu = n - 1$ and $\mu = n$.

The same boundary equation appears when one considers self-consistency equation for the order parameter, $\psi = \langle \psi_{gs} | b | \psi_{gs} \rangle$. First order correction to the wave function enables to find the first term (linear in ψ) in the expansion $\langle \psi_{gs} | b | \psi_{gs} \rangle = t\psi\chi_0 + \dots$, where higher order terms in ψ will come out if one takes into account next order corrections to the wave function. The critical boundary corresponds to the vanishing of the coefficient of the term linear in ψ , which amounts to $\psi = t\psi\chi_0$, and one obtains the same boundary equation.

By construction the standard mean-field scheme cannot describe the degenerate character of the ground state in the two extremes $\mu = n - 1$ and $\mu = n$ since it is based on the consideration of interval $n - 1 < \mu < n$ and implicitly involves, at $t = 0$, $|\psi_{gs}\rangle = |n\rangle$ as the reference state. The corresponding Eqs. (5), (6) and (7) have singularities at $\mu = n - 1, n$.

Below we show how to change the perturbation expansion to account for the degenerate case with integers values of μ . This approach let us identify the phase boundary of the insulating lobes with no divergence in resulting expressions. Though the resulting equation for the critical boundary will be the same as Eq. (8) this approach provide us information on the behavior of the order parameter in the superfluid phase.

The basic idea is to make first diagonalization of the perturbation in two dimensional subspace spanned by vectors $\mathcal{P}_n^2 = \{|n\rangle, |n+1\rangle\}$. It is supposed that the value of μ should lie in certain interval around $\mu = n$ so that ε_n and ε_{n+1} are the only two lowest energies of h_0 . Below it is convenient to set $\mu = n + \delta$. Then at $1/2 \leq \delta < 1$ the lowest energies are $\varepsilon_{n+1} < \varepsilon_{n+2} \leq \varepsilon_n$, while at $-1 < \delta \leq -1/2$ the lowest energies are $\varepsilon_n < \varepsilon_{n-1} \leq \varepsilon_{n+1}$. Therefore, the value of δ is supposed to lie in the segment $-1/2 < \delta < 1/2$. At integer $\mu = n$ this approach accounts for the degenerate level with $\varepsilon_n = \varepsilon_{n+1}$.

We introduce a projection operator P onto the subspace \mathcal{P}_n^2 and its orthogonal completion P^\perp

$$P = |n\rangle\langle n| + |n+1\rangle\langle n+1|, \quad P^\perp = 1 - P \quad (9)$$

and rewrite the perturbation as

$$h_t = h'_t + h''_t, \quad (10)$$

$$h'_t = Ph_tP, \quad h''_t = Ph_tP^\perp + P^\perp h_tP + P^\perp h_tP^\perp \quad (11)$$

The term h'_t we include into $\tilde{h}_0 = h_0 + h'_t$ and the term h''_t we shall treat as a new perturbation. Upon performing the exact diagonalization of \tilde{h}_0 in the two-dimensional subspace \mathcal{P}_n^2 ,

$$\tilde{h}_0 = \begin{pmatrix} \varepsilon_n & -t\psi^*\sqrt{n+1} \\ -t\psi\sqrt{n+1} & \varepsilon_{n+1} \end{pmatrix}, \quad (12)$$

one obtains two new zero-order wave functions $|\psi_a^{(0)}\rangle$ (for lower level) and $|\psi_b^{(0)}\rangle$ (for upper level)

$$|\psi_a^{(0)}\rangle = C_1|n\rangle + C_2|n+1\rangle, \quad (13)$$

$$|\psi_b^{(0)}\rangle = C'_1|n\rangle + C'_2|n+1\rangle, \quad (14)$$

where normalized coefficients are

$$|C_1|^2 = \frac{1}{2} \left(1 - \frac{\delta}{\Delta E} \right), \quad |C_2|^2 = \frac{1}{2} \left(1 + \frac{\delta}{\Delta E} \right), \quad (15)$$

$$|C'_1|^2 = \frac{1}{2} \left(1 + \frac{\delta}{\Delta E} \right), \quad |C'_2|^2 = \frac{1}{2} \left(1 - \frac{\delta}{\Delta E} \right) \quad (16)$$

The corresponding energy levels are ($E_a < E_b$)

$$E_a = \varepsilon_n - \frac{1}{2}(\Delta E + \delta), \quad E_b = \varepsilon_n + \frac{1}{2}(\Delta E - \delta), \quad (17)$$

The value of E_a gives the energy of the ground state of the Hamiltonian \tilde{h}_0 . Here $\Delta E = \sqrt{\delta^2 + 4t^2|\psi|^2(n+1)}$ is the splitting between the two states, $E_b - E_a = \Delta E \geq |\delta|$, and $\delta = \mu - n = \varepsilon_n - \varepsilon_{n+1}$, $-1/2 < \delta < 1/2$. In the Mott phase $|\psi| = 0$, the corresponding ground state wave function is either $|\psi_a^{(0)}\rangle = |n+1\rangle$ for positive $\delta > 0$ ($\Delta E = \delta$), or $|\psi_a^{(0)}\rangle = |n\rangle$ for negative $\delta < 0$ ($\Delta E = -\delta$).

At integer values of μ ($\mu = n$, $\delta = 0$) the splitting is proportional to the magnitude of the order parameter, $\Delta E = 2t|\psi|\sqrt{n+1}$. To this non-analytical dependence of ground state energy on ψ at integer values of μ , $E_{gs} = t|\psi|^2 + E_a = -n(n+1)/2 + t|\psi|^2 - t|\psi|\sqrt{n+1}$, was pointed out in Ref. [10].

According to the standard perturbation theory the first order correction to the ground state wave function is

$$|\psi_a^{(1)}\rangle = \sum_{k \neq n, n+1} \frac{\langle k | h''_t | \psi_a^{(0)} \rangle}{E_a - \varepsilon_k} |k\rangle \quad (18)$$

Of three terms of h''_t , Eq. (10), only term $P^\perp h_t P$ gives a contribution into matrix element $\langle k | h''_t | \psi_a^{(0)} \rangle$. As a result the perturbed wave function is

$$\begin{aligned} |\psi_a\rangle &= |\psi_a^{(0)}\rangle + |\psi_a^{(1)}\rangle = \\ &= C_1|n\rangle + C_2|n+1\rangle + \\ &+ C_1 \frac{(-t)\psi^*\sqrt{n}}{E_a - \varepsilon_{n-1}} |n-1\rangle + C_2 \frac{(-t)\psi\sqrt{n+2}}{E_a - \varepsilon_{n+2}} |n+2\rangle \end{aligned} \quad (19)$$

Comparing Eqs. (5) and (19) one can clearly see the advantage of this approach, namely the coefficients of the decomposition of $|\psi_a\rangle$ have regular behavior as functions of μ .

Self-consistency equation for the order parameter, $\psi = \langle \psi_a | b | \psi_a \rangle$, is reduced to equation

$$\psi = t\psi\chi_a, \quad \chi_a = \frac{1}{\Delta E} \left[(n+1) + n \frac{\Delta E - \delta}{2 + 3\delta + \Delta E} + (n+2) \frac{\Delta E + \delta}{2 - 3\delta + \Delta E} \right] \quad (20)$$

Close to the critical boundary, $|\psi|^2 \simeq 0$, Eq. (20) can be rewritten as

$$\psi = \begin{cases} t\psi\chi_0(\mu, n+1), & \delta > 0, \\ t\psi\chi_0(\mu, n), & \delta < 0 \end{cases} \quad (21)$$

Eq. (21) gives the lower part of the lobe $\mu(t, n+1)$ at $n \leq \mu \leq n+1/2$ and the upper part of the lobe $\mu(t, n)$ at $n-1/2 \leq \mu \leq n$. Combining parts from different n results in standard mean-field lobes as described by Eq. (8).

Another way to obtain the position of the phase boundary in the plane (μ, t) is to consider a correction to the ground state energy. It is a sum of three terms, $\Delta E_{gs} = t|\psi|^2 + (E_a - E_{gs}^{(0)}) + \Delta E_{gs}^{(2)}$, $E_{gs}^{(0)} = \min(\varepsilon_n, \varepsilon_{n+1})$, originating from: (i) the mean-field treatment of the hopping term, (ii) a correction due to the formation of the state $|\psi_a^{(0)}\rangle$, $E_a - E_{gs}^{(0)} \simeq -t^2|\psi|^2(n+1)/\Delta E$, and (iii) the second order correction due to the perturbation h_t'' ,

$$\begin{aligned} \Delta E_{gs}^{(2)} &= t^2|\psi|^2 \left[\frac{|C_1|^2 n}{E_a - \varepsilon_{n-1}} + \frac{|C_2|^2 (n+2)}{E_a - \varepsilon_{n+2}} \right] = \\ &= -t^2|\psi|^2 \frac{1}{\Delta E} \left[n \frac{(\Delta E - \delta)}{2 + 3\delta + \Delta E} + (n+2) \frac{(\Delta E + \delta)}{2 - 3\delta + \Delta E} \right] \end{aligned} \quad (22)$$

Gathering all three terms one obtains the correction to the ground state energy, $\Delta E_{gs} = t|\psi|^2(1 - t\chi_a)$, where χ_a is given by Eq. (20). At the phase boundary, $\Delta E = |\delta|$, and $\chi_a = \chi_0(\mu, n+1)$ at $\delta > 0$, or $\chi_a = \chi_0(\mu, n)$ at $\delta < 0$. One recovers the upper and lower parts of the corresponding lobes.

From Eq. (20) one enables also obtain some qualitative information about the behavior of order parameter in the superfluid phase. Namely, one can recover the dependence of the order parameter $|\psi|^2$ on parameters μ and t . This dependence is shown in Fig. 1. Mott insulating lobes (thick lines) coincide with the prediction of standard perturbation approach, Eq. (8). Thin lines outside the insulating lobes correspond to a few contours of $|\psi|^2 = \text{const}$ inside the superfluid phase.

The contour plot is discontinuous at points corresponding to half-integer values of μ . This can be expected from our restriction of the Hamiltonian h_t to the two-dimensional subspace \mathcal{P}_n^2 . By going from \mathcal{P}_n^2 to another

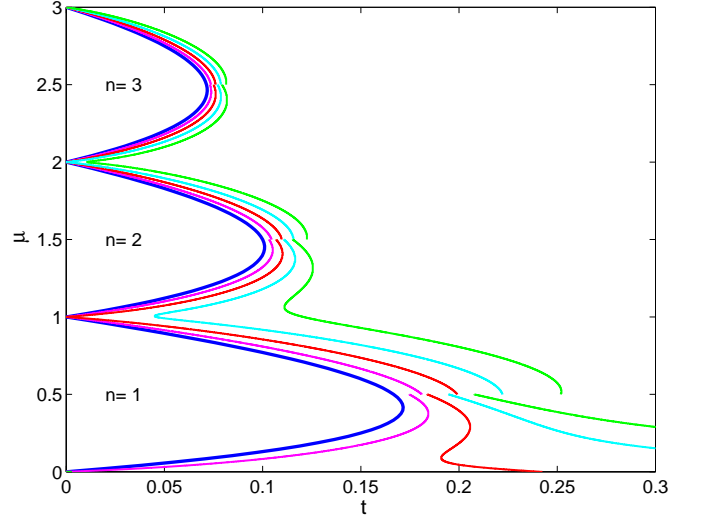


FIG. 1: Mean- field phase diagram for the BH model (3). Thick lines indicate the Mott insulating lobes for $n = 1, 2$ and 3. Thin lines are contours of constant value of the order parameter, corresponding to $|\psi|^2 = 0.2, 0.4, 0.6$ and 0.8.

\mathcal{P}_{n+1}^2 matrix elements of the restricted perturbation h_t' jump to new values. This artificial feature can be circumvented if to use the bigger vector space of number states $\{|n\rangle\}$, $n = 0, 1, \dots, n_{max}$. Then it will be equivalent to the approach of Refs. [8, 34].

In summary, we presented an alternative way to estimate perturbation corrections to the ground state wave function of the mean field BH Hamiltonian (3). This approach has an advantage that the corrections to $|\psi_{gs}\rangle$ and E_{gs} do not have singularities at integer values of the chemical potential. It enables, as well, to describe the behavior of $|\psi|$ also in the superfluid phase. However, the restriction of the perturbation onto the two-dimensional subspace \mathcal{P}_n^2 introduces the discontinuity in the behavior of order parameter $|\psi|$ at half-integer values of μ in the superfluid phase.

The fact that one obtains the same equation for critical boundary, $t = 1/\chi_0(\mu, n)$, using degenerate and non-degenerate (standard) perturbation expansion tells that this equation is the generic property of the on-site mean-field approximation and is not connected with the way how one take into account degeneracy of spectrum ε_n at integers values of μ .

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- A.S. De and U. Sen, Adv. Phys. **56**, 243 (2007).
- [3] P.B. Weichman, Mod. Phys. Lett. B **22**, 2623 (2008).
- [4] M. Greiner, O. Mandel, T. Esslinger, T. Hänsch, I. Bloch, Nature **415**, 39 (2002).
- [5] M.P.A. Fisher, P.B. Weichman, G. Grinstein, D.S. Fisher, Phys. Rev. B **40**, 546 (1989).
- [6] D. Rokhsar, B.G. Kotliar, Phys. Rev. B **44**, 10328 (1991).
- [7] W. Krauth, M. Caffarel, J.P. Bouchaud, Phys. Rev. B **45**, 3137 (1992).
- [8] D. Jaksch, C. Bruder, J.I. Cirac, C.W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
- [9] K. Sheshadri, H.R. Krishnamurthy, R. Pandit and T.V. Ramakrishnan, Europhys. Lett. **22**, 257 (1993).
- [10] D. van Oosten, P. van der Straten, and H.T.C. Stoof, Phys. Rev. A **63**, 053601 (2001).
- [11] V.A. Kashurnikov, N.V. Prokof'ev, and B.V. Svistunov, Phys. Rev. A **66**, 031601 (2002).
- [12] F. Alet, E. Sørensen, Phys. Rev. B **70**, 024513 (2004).
- [13] B. Capogrosso-Sansone, N.V. Prokof'ev, and B.V. Svistunov, Phys. Rev. A **75**, 134302 (2007).
- [14] M. Capello, M. Becca, M. Fabrizio, S. Sorella, Phys. Rev. Lett. **99**, 056402 (2007).
- [15] D.-S. Lühmann, Phys. Rev. A **87**, 043619 (2013).
- [16] J.K. Freericks and H. Monien, Phys. Rev. B **53**, 2691 (1996); J.K. Freericks, H.R. Krishnamurthy, Y. Kato, N. Kawashima, and N. Trivedi, Phys. Rev. A **79**, 053631 (2009).
- [17] K. Ziegler, Europhys. Lett. **23**, 463 (1993).
- [18] R. Fresard, e-print cond-mat/9405053.
- [19] D.B.M. Dickerscheid, D. van Oosten, P.J.H. Denteneer, and H.T.C. Stoof, Phys. Rev. A **68**, 043623 (2003).
- [20] K. Sengupta, N. Dupuis, Phys. Rev. A **71**, 033629 (2005); N. Dupuis, K. Sengupta, Physica B **404**, 517 (2009).
- [21] F.E.A. dos Santos, A. Pelster, Phys. Rev. A **79**, 013614 (2009).
- [22] B. Bradlyn, F.E.A. dos Santos, A. Pelster, Phys. Rev. A **79**, 013615 (2009).
- [23] Y. Ohashi, M. Kitaura, and H. Matsumoto, Phys. Rev. A **73**, 033617 (2006).
- [24] S. Konabe, T. Nikuni, and M. Nakamura, Phys. Rev. A **73**, 033621 (2006).
- [25] C. Menotti, N. Trivedi, Phys. Rev. B **77**, 235120 (2008).
- [26] A. Kauch, K. Byczuk, D. Vollhardt, Phys. Rev. B **85**, 205115 (2012).
- [27] P. Buonsante, V. Penna, A. Vezzani, Phys. Rev. A **70**, 061603(R) (2004).
- [28] P. Buonsante, V. Penna, A. Vezzani, Laser Physics **15**, 361 (2005).
- [29] T. McIntosh, P. Pisarski, R.J. Gooding, and E. Zaremba, Phys. Rev. A **86**, 013623 (2012).
- [30] A. Eckardt, Phys. Rev. A **79**, 195131 (2009).
- [31] N. Teichmann, D. Hinrichs, M. Holthaus, A. Eckardt, Phys. Rev. A **79**, 224515 (2009).
- [32] R.A. Barankov, C. Lannert, and A. Vishveshwara, Phys. Rev. A **75**, 063622 (2007).
- [33] K. Sun, C. Lannert, and A. Vishveshwara, Phys. Rev. A **79**, 043422 (2009).
- [34] C. Trefzger, C. Menotti, and M. Lewenstein, Phys. Rev. A **78**, 043604 (2008).
- [35] S. Sachdev, Quantum Phase Transitions, Cambridge University Press, Cambridge, England, 1999.